

FILE LAST UPDATED: 9 Jul 2003 . (20030709/ED)

HCAPLUS COPYRIGHT 2003 ACS

AN 1992:83328 HCAPLUS Full-text

DN 116:83328

TI A novel class of enkephalinase inhibitors containing a C-terminal sulfo group

AU Mimura, Tetsutaro; Nakamura, Yasuhisa; Nishino, Junko; Sawayama, Tadahiro; Komiya, Toshio; Deguchi, Takashi; Kita, Atsuko; Nakamura, Hideo; Matsumoto, Junichi

CS Res. Lab., Dainippon Pharm. Co., Ltd., Suita, 564, Japan

SO **Journal of Medicinal Chemistry** (1992), 35(3), 602-8

CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 1

OS CASREACT 116:83328

AB A series of β -aryl-N-(sulfoalkyl)- α -(thiomethyl)propionamides and β -aryl-N-(sulfoaryl)- α -(thiomethyl)propionamides were prepd. and tested as enkephalinase and angiotensin-converting enzyme inhibitors. The enkephalinase-inhibiting activity (IC₅₀) of β -phenyl-(3-sulfophenyl)- α -(thiomethyl)propionamide was 0.27 nM; several analogs had an IC comparable to thiorphan. β -Phenyl-(2-sulfoethyl)- α -(thiomethyl)propionamide was tested for analgesic activity.

ST arylsulfoalkylthiomethyl propionamide enkephalinase inhibitor;
propionamide arylsulfoalkylthiomethyl enkephalinase inhibitor;
enkephalinase inhibitor arylsulfoalkylthiomethyl propionamide; angiotensin converting enzyme arylsulfoalkylthiomethyl propionamide; analgesic arylsulfoalkylthiomethyl propionamide; phenylsulfoethylthiomethyl propionamide analgesic

IT Analgesics

(aryl(thiomethyl)-N-(sulfoalkyl)propionamides as)

IT Molecular structure-biological activity relationship

(enkephalin dipeptidyl carboxypeptidase-inhibiting, of
(aryl(thiomethyl)-N-(sulfoalkyl)propionamides as)

IT Enzymes

RL: USES (Uses)

(enkephalin-degrading, inhibitors, aryl(thiomethyl)-N-(sulfoalkyl)propionamides as)

IT 105-53-3, Diethyl malonate

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation of, with aryl bromides or iso-Pr bromide, conversion to acrylic acid deriv., and sequential condensation with thioacetic acid of)

IT 78-77-3 100-11-8, 4-Nitrobenzyl bromide 100-39-0, Benzyl bromide
104-81-4, 4-Methylbenzyl bromide 402-49-3, 4-(Trifluoromethyl)benzyl
bromide 459-46-1, 4-Fluorobenzyl bromide 637-59-2 2567-29-5
3163-27-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(alkylation with, of di-Et malonate)

IT 9015-82-1, Angiotensin-converting enzyme 70025-49-9

RL: USES (Uses)

(inhibitors, (arylmethyl)(thiomethyl)-N-(sulfoalkyl)propionamides as)

IT 58353-47-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and conversion of, to (acetylthio)(aminobenzyl)propionic acid)

IT 116111-78-5P 116111-88-7P 116111-90-1P 116112-04-0P 116112-13-1P
116112-14-2P 116112-18-6P 116112-19-7P 116112-21-1P 116112-22-2P
116112-23-3P 116112-24-4P 116112-25-5P 116112-26-6P 116112-29-9P
116112-32-4P 116112-33-5P 116112-34-6P 116112-36-8P 116112-37-9P
116112-38-0P 116112-39-1P 116112-41-5P 126772-38-1P 126772-42-7P
126772-44-9P 126772-46-1P 126795-60-6P 138062-99-4P 138063-00-0P
138063-01-1P 138063-02-2P 138063-15-7P 138063-17-9P 138063-18-0P

138063-19-1P 138063-22-6P 138063-27-1P 138063-29-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (prepn. and deacetylation of)

IT 76789-49-6P 82154-12-9P **115355-28-7P** 116112-43-7P
 116112-46-0P 116112-47-1P 116112-48-2P 116112-49-3P 123829-77-6P
123986-61-8P 138062-89-2P **138062-93-8P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and resolu. and conversion of, to aryl-N-
 (sulfoalkyl)(thiomethyl)propionamide)

IT 91702-98-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and resolu. and conversion of, to phenyl-N-
 (sulfoalkyl)(thiomethyl)propionamide)

IT 116111-79-6P 124815-67-4P 138062-84-7P 138062-85-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

IT 116111-85-4P 116112-03-9P 116112-08-4P 116112-09-5P 116112-11-9P
 138063-30-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as enkephalinase and angiotensin-converting enzyme
 inhibitor)

IT 116111-86-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as enkephalinase and angiotensin-converting enzyme
 inhibitor and analgesic)

IT 116111-82-1P 116111-91-2P 116111-92-3P 116111-93-4P 116111-94-5P
 116111-97-8P 116111-98-9P 116112-00-6P 116112-01-7P 116112-05-1P
 116112-06-2P 116112-10-8P 116155-52-3P 126772-36-9P 126772-39-2P
 126772-43-8P 126772-45-0P 126772-47-2P 138063-34-0P 138063-35-1P
 138063-36-2P 138063-37-3P 138063-41-9P 138063-50-0P 138063-53-3P
 138063-54-4P 138063-56-6P 138063-57-7P 138063-62-4P 138063-64-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, as enkephalinase inhibitor)

IT 107-35-7, Taurine 121-57-3, Sulfanilic acid
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with (acetylthio)benzylpropionic acid)

IT 507-09-5, Thioacetic acid, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with acrylic acid derivs.)

IT 100-10-7, 4-(Dimethylamino)benzaldehyde 123-11-5, 4-Methoxybenzaldehyde,
 reactions 500-22-1, 3-Pyridinecarboxaldehyde 37924-85-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with di-Et malonate)

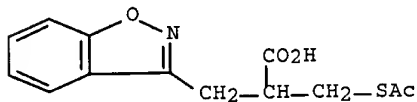
* * * * * Welcome to STN International * * * * *

FILE 'REGISTRY' ENTERED AT 11:41:58 ON 11 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 9 JUL 2003 HIGHEST RN 545225-95-4
DICTIONARY FILE UPDATES: 9 JUL 2003 HIGHEST RN 545225-95-4

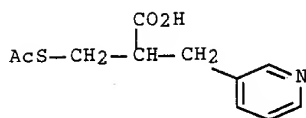
L1 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2003 ACS
RN **138062-93-8** REGISTRY
CN 1,2-Benzisoxazole-3-propanoic acid, α -[(acetylthio)methyl]-, sodium
salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1,2-Benzisoxazole-3-propanoic acid, α -[(acetylthio)methyl]-, sodium
salt, (\pm)-
MF C13 H13 N O4 S . Na
SR CA
LC STN Files: CA, CAPLUS
CRN (126772-53-0)



● Na

1 REFERENCES IN FILE CA (1957 TO DATE)
1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

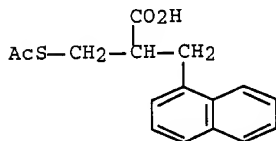
L1 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2003 ACS
RN 123986-61-8 REGISTRY
CN 3-Pyridinepropanoic acid, α -[(acetylthio)methyl]- (9CI) (CA INDEX
NAME)
OTHER NAMES:
CN 2-(Acetylthiomethyl)-3-(3-pyridinyl)propionic acid
FS 3D CONCORD
DR **138062-92-7**
MF C11 H13 N O3 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1957 TO DATE)
6 REFERENCES IN FILE CAPLUS (1957 TO DATE)

L1 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2003 ACS
RN 115355-28-7 REGISTRY
CN 1-Naphthalenepropanoic acid, α -[(acetylthio)methyl]- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 2-(Acetylthiomethyl)-3-(1-naphthyl)propionic acid
FS 3D CONCORD
DR **138062-91-6**
MF C16 H16 O3 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, USPATFULL
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1957 TO DATE)
5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

FILE 'HCAPLUS' ENTERED AT 11:43:18 ON 11 JUL 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 11 Jul 2003 VOL 139 ISS 2